Supporting Information for Publication: Computation of Molecular Electron Affinities using an Ensemble Density Functional Theory Method

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1 Dyson's orbitals from Table 1 of the main article obtained with the 6-31G* basis set

Table S1: Electron attachment Dyson's orbitals calculated using the 6-31G* basis set. See legend to Table 1 of the main article for detail.

Molecule	EKT-SSR-BH&HLYP		RBH&HLYP	
	$-\varepsilon_1^D$	$-\varepsilon_2^D$	$-\varepsilon_{LUMO}$	$-\varepsilon_{LUMO+1}$
naphthalene	-0.27	-1.10	-0.26	-1.09
anthracene	0.51	-0.90	0.52	-0.90
tetracene	1.04	-0.77	1.05	-0.77
pentacene	1.42	-0.29	1.42	-0.29
pyrene	0.38	-0.54	0.39	-0.54
phenanthrene	-0.21	-0.36	-0.20	-0.36
perylene	0.84	-0.76	0.85	-0.76
picene	0.10	0.04	0.11	0.04
chrysene	0.11	-0.32	0.12	-0.32
fluoranthene	0.64	-0.74	0.65	-0.74
azulene	0.66	0.13	0.72	0.10
C_2H_4	-1.97	-4.64	-2.01	-4.64
C_2H_3F	-1.88	-4.44	-1.92	-4.44
1,1-$C_2H_2F_2$	-1.89	-4.46	-1.84	-4.40
trans-$C_2H_2F_2$	-1.68	-3.57	-1.63	-3.56
cis-$C_2H_2F_2$	-1.75	-3.56	-1.71	-3.55
C_2HF_3	-1.68	-3.32	-1.62	-3.28
C_2F_4	-1.59	-3.18	-1.51	-3.17
pyridine	-0.79	-1.11	-0.82	-1.09
butadiene	-0.83	-4.01	-0.82	-4.01
1,3-cyclohexadiene	-0.95	-3.86	-0.95	-3.86
furan	-2.04	-3.77	-2.01	-3.76
thiophene	-1.13	-2.42	-1.13	-2.42
MAD[a)]	0.31		0.31	

[a)] Mean absolute deviation (in eV) from the experimental electron affinities reported in Table 1 of the main article.

2 Linear regression analysis of Eq. (6) of the main article

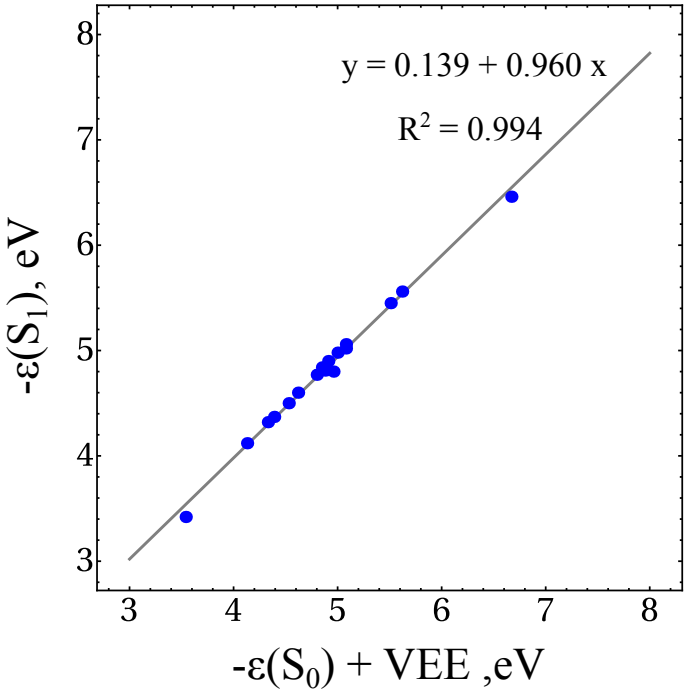

Figure S1: Linear regression analysis of Eq. (6) reported in the main article. Blue dots show the most positive electron affinities reported in Tables 1 and 2 of the main article.

3 Cartesian coordinates of all molecules studied in the main paper

Table S2: Geometries (in Å) of all the molecules reported in the main article. The geometries were optimized using the SSR-BH&HLYP/6-311G** method.

Molecule	Atom	X	Y	Z
naphthalene				
	C	0.000000	1.237790	1.392371
	C	0.000000	2.415924	0.705121
	C	0.000000	2.415924	-0.705121
	C	0.000000	1.237790	-1.392371
	C	0.000000	-1.237790	-1.392371
	C	0.000000	-2.415924	-0.705121
	C	0.000000	-2.415924	0.705121
	C	0.000000	-1.237790	1.392371
	C	0.000000	0.000000	0.708734
	C	0.000000	0.000000	-0.708734
	H	0.000000	1.233988	2.471178
	H	0.000000	3.353602	1.236820
	H	0.000000	3.353602	-1.236820
	H	0.000000	1.233988	-2.471178
	H	0.000000	-1.233988	-2.471178
	H	0.000000	-3.353602	-1.236820
	H	0.000000	-3.353602	1.236820
	H	0.000000	-1.233988	2.471178
anthracene				
	C	0.000000	3.633733	0.710816
	C	0.000000	3.633733	-0.710816
	C	0.000000	2.464681	-1.397677
	C	0.000000	2.464681	1.397677
	H	0.000000	2.461226	-2.476342
	H	0.000000	2.461226	2.476342
	C	0.000000	1.213506	-0.715174
	C	0.000000	1.213506	0.715174
	C	0.000000	0.000000	1.392890
	C	0.000000	0.000000	-1.392890
	H	0.000000	0.000000	2.472272
	H	0.000000	0.000000	-2.472272
	C	0.000000	-1.213506	0.715174
	C	0.000000	-1.213506	-0.715174
	C	0.000000	-2.464681	-1.397677
	C	0.000000	-2.464681	1.397677
	H	0.000000	-2.461226	-2.476342

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	H	0.000000	-2.461226	2.476342
	C	0.000000	-3.633733	-0.710816
	C	0.000000	-3.633733	0.710816
	H	0.000000	-4.573626	1.238487
	H	0.000000	-4.573626	-1.238487
	H	0.000000	4.573626	1.238487
	H	0.000000	4.573626	-1.238487
tetracene				
	C	0.000000	4.852890	0.713724
	C	0.000000	4.852890	-0.713724
	C	0.000000	3.688203	-1.400768
	C	0.000000	3.688203	1.400768
	H	0.000000	3.685131	-2.479376
	H	0.000000	3.685131	2.479376
	C	0.000000	2.430470	-0.719272
	C	0.000000	2.430470	0.719272
	C	0.000000	1.228085	1.395959
	C	0.000000	1.228085	-1.395959
	H	0.000000	1.227713	2.475197
	H	0.000000	1.227713	-2.475197
	C	0.000000	0.000000	0.718326
	C	0.000000	0.000000	-0.718326
	C	0.000000	-1.228085	-1.395959
	C	0.000000	-1.228085	1.395959
	H	0.000000	-1.227713	-2.475197
	H	0.000000	-1.227713	2.475197
	C	0.000000	-2.430470	-0.719272
	C	0.000000	-2.430470	0.719272
	C	0.000000	-3.688203	1.400768
	C	0.000000	-3.688203	-1.400768
	H	0.000000	-3.685131	2.479376
	H	0.000000	-3.685131	-2.479376
	C	0.000000	-4.852890	0.713724
	C	0.000000	-4.852890	-0.713724
	H	0.000000	-5.793913	-1.239391
	H	0.000000	-5.793913	1.239391
	H	0.000000	5.793913	-1.239391
	H	0.000000	5.793913	1.239391
pentacene				
	C	0.000000	4.910187	1.402452
	C	0.000000	4.910187	-1.402452
	H	0.000000	4.907386	2.481048
	H	0.000000	4.907386	-2.481048
	C	0.000000	6.072542	0.715384

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	C	0.000000	6.072542	-0.715384
	C	0.000000	3.649026	0.721715
	C	0.000000	3.649026	-0.721715
	C	0.000000	2.452349	-1.397886
	C	0.000000	2.452349	1.397886
	H	0.000000	2.452038	-2.477088
	H	0.000000	2.452038	2.477088
	C	0.000000	1.216190	-0.721019
	C	0.000000	1.216190	0.721019
	C	0.000000	0.000000	1.397947
	C	0.000000	0.000000	-1.397947
	H	0.000000	0.000000	2.477037
	H	0.000000	0.000000	-2.477037
	C	0.000000	-1.216190	0.721019
	C	0.000000	-1.216190	-0.721019
	C	0.000000	-2.452349	-1.397886
	C	0.000000	-2.452349	1.397886
	H	0.000000	-2.452038	-2.477088
	H	0.000000	-2.452038	2.477088
	C	0.000000	-3.649026	-0.721715
	C	0.000000	-3.649026	0.721715
	C	0.000000	-4.910187	1.402452
	C	0.000000	-4.910187	-1.402452
	H	0.000000	-4.907386	2.481048
	H	0.000000	-4.907386	-2.481048
	C	0.000000	-6.072542	0.715384
	C	0.000000	-6.072542	-0.715384
	H	0.000000	7.014266	-1.239703
	H	0.000000	7.014266	1.239703
	H	0.000000	-7.014266	-1.239703
	H	0.000000	-7.014266	1.239703
pyrene				
	C	0.000000	-3.498843	0.000000
	C	0.000000	-2.812738	1.202518
	C	0.000000	-1.420025	1.224881
	C	0.000000	-0.711128	0.000000
	C	0.000000	-1.420025	-1.224881
	C	0.000000	-2.812738	-1.202518
	C	0.000000	-0.673612	2.449111
	C	0.000000	0.711128	0.000000
	C	0.000000	1.420025	1.224881
	C	0.000000	0.673612	2.449111
	C	0.000000	2.812738	1.202518
	H	0.000000	3.355413	2.135149

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	C	0.000000	3.498843	0.000000
	C	0.000000	2.812738	-1.202518
	C	0.000000	1.420025	-1.224881
	H	0.000000	-1.218665	3.379393
	H	0.000000	-4.576609	0.000000
	H	0.000000	-3.355413	2.135149
	H	0.000000	-3.355413	-2.135149
	H	0.000000	1.218665	3.379393
	H	0.000000	4.576609	0.000000
	H	0.000000	3.355413	-2.135149
	C	0.000000	0.673612	-2.449111
	C	0.000000	-0.673612	-2.449111
	H	0.000000	1.218665	-3.379393
	H	0.000000	-1.218665	-3.379393
phenanthrene				
	C	0.000000	-3.537068	-0.293828
	C	0.000000	-2.819419	0.872379
	C	0.000000	-1.413906	0.857107
	C	0.000000	-0.725895	-0.375896
	C	0.000000	-1.490243	-1.556362
	C	0.000000	-2.861218	-1.518792
	C	0.000000	-0.673161	2.080612
	C	0.000000	0.725895	-0.375896
	C	0.000000	1.413906	0.857107
	C	0.000000	0.673161	2.080612
	C	0.000000	2.819419	0.872379
	H	0.000000	3.327126	1.824451
	C	0.000000	3.537068	-0.293828
	C	0.000000	2.861218	-1.518792
	C	0.000000	1.490243	-1.556362
	H	0.000000	-1.220016	3.010006
	H	0.000000	-4.614633	-0.270737
	H	0.000000	-3.327126	1.824451
	H	0.000000	-1.000997	-2.514928
	H	0.000000	-3.420008	-2.440117
	H	0.000000	1.220016	3.010006
	H	0.000000	4.614633	-0.270737
	H	0.000000	3.420008	-2.440117
	H	0.000000	1.000997	-2.514928
perylene				
	C	-2.408625	1.468456	0.000000
	C	-1.242413	0.736501	0.000000
	C	0.000000	1.433201	0.000000
	C	0.000000	2.853478	0.000000

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	C	-1.225372	3.551924	0.000000
	C	-2.404604	2.869323	0.000000
	H	-3.361484	0.970270	0.000000
	C	1.242413	0.736501	0.000000
	C	1.225372	3.551924	0.000000
	H	-1.208936	4.630066	0.000000
	H	-3.343177	3.399274	0.000000
	C	2.404604	2.869323	0.000000
	C	2.408625	1.468456	0.000000
	H	1.208936	4.630066	0.000000
	H	3.343177	3.399274	0.000000
	H	3.361484	0.970270	0.000000
	C	-2.404604	-2.869323	0.000000
	C	-1.225372	-3.551924	0.000000
	C	0.000000	-2.853478	0.000000
	C	0.000000	-1.433201	0.000000
	C	-1.242413	-0.736501	0.000000
	C	-2.408625	-1.468456	0.000000
	H	1.208936	-4.630066	0.000000
	H	-3.343177	-3.399274	0.000000
	H	-1.208936	-4.630066	0.000000
	C	1.225372	-3.551924	0.000000
	C	1.242413	-0.736501	0.000000
	H	-3.361484	-0.970270	0.000000
	C	2.408625	-1.468456	0.000000
	C	2.404604	-2.869323	0.000000
	H	3.361484	-0.970270	0.000000
	H	3.343177	-3.399274	0.000000
picene				
	C	0.000000	-5.683809	-0.381267
	C	0.000000	-4.969898	0.785261
	C	0.000000	-3.562918	0.771490
	C	0.000000	-2.870062	-0.457961
	C	0.000000	-3.634258	-1.641719
	C	0.000000	-5.003845	-1.606494
	C	0.000000	-2.817980	1.983887
	C	0.000000	-1.422899	-0.453372
	C	0.000000	-0.719257	0.762277
	C	0.000000	-1.468455	1.980246
	C	0.000000	0.719257	0.762277
	C	0.000000	1.422899	-0.453372
	C	0.000000	0.678116	-1.656705
	C	0.000000	-0.678116	-1.656705
	H	0.000000	-3.356143	2.918942

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	H	0.000000	-6.761441	-0.361410
	H	0.000000	-5.477129	1.737530
	H	0.000000	-3.146211	-2.600247
	H	0.000000	-5.560331	-2.529493
	H	0.000000	-0.955376	2.924015
	H	0.000000	1.187853	-2.603203
	H	0.000000	-1.187853	-2.603203
	C	0.000000	2.870062	-0.457961
	C	0.000000	3.562918	0.771490
	C	0.000000	2.817980	1.983887
	C	0.000000	1.468455	1.980246
	H	0.000000	3.356143	2.918942
	H	0.000000	0.955376	2.924015
	C	0.000000	3.634258	-1.641719
	C	0.000000	5.003845	-1.606494
	C	0.000000	5.683809	-0.381267
	C	0.000000	4.969898	0.785261
	H	0.000000	3.146211	-2.600247
	H	0.000000	5.560331	-2.529493
	H	0.000000	6.761441	-0.361410
	H	0.000000	5.477129	1.737530
chrysene				
	C	-2.408625	1.468456	0.000000
	C	-1.242413	0.736501	0.000000
	C	0.000000	1.433201	0.000000
	C	0.000000	2.853478	0.000000
	C	-1.225372	3.551924	0.000000
	C	-2.404604	2.869323	0.000000
	H	-3.361484	0.970270	0.000000
	C	1.242413	0.736501	0.000000
	C	1.225372	3.551924	0.000000
	H	-1.208936	4.630066	0.000000
	H	-3.343177	3.399274	0.000000
	C	2.404604	2.869323	0.000000
	C	2.408625	1.468456	0.000000
	H	1.208936	4.630066	0.000000
	H	3.343177	3.399274	0.000000
	H	3.361484	0.970270	0.000000
	C	-2.404604	-2.869323	0.000000
	C	-1.225372	-3.551924	0.000000
	C	0.000000	-2.853478	0.000000
	C	0.000000	-1.433201	0.000000
	C	-1.242413	-0.736501	0.000000
	C	-2.408625	-1.468456	0.000000

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	H	1.208936	-4.630066	0.000000
	H	-3.343177	-3.399274	0.000000
	H	-1.208936	-4.630066	0.000000
	C	1.225372	-3.551924	0.000000
	C	1.242413	-0.736501	0.000000
	H	-3.361484	-0.970270	0.000000
	C	2.408625	-1.468456	0.000000
	C	2.404604	-2.869323	0.000000
	H	3.361484	-0.970270	0.000000
	H	3.343177	-3.399274	0.000000
fluoranthene				
	C	-2.408625	1.468456	0.000000
	C	-1.242413	0.736501	0.000000
	C	0.000000	1.433201	0.000000
	C	0.000000	2.853478	0.000000
	C	-1.225372	3.551924	0.000000
	C	-2.404604	2.869323	0.000000
	H	-3.361484	0.970270	0.000000
	C	1.242413	0.736501	0.000000
	C	1.225372	3.551924	0.000000
	H	-1.208936	4.630066	0.000000
	H	-3.343177	3.399274	0.000000
	C	2.404604	2.869323	0.000000
	C	2.408625	1.468456	0.000000
	H	1.208936	4.630066	0.000000
	H	3.343177	3.399274	0.000000
	H	3.361484	0.970270	0.000000
	C	-2.404604	-2.869323	0.000000
	C	-1.225372	-3.551924	0.000000
	C	0.000000	-2.853478	0.000000
	C	0.000000	-1.433201	0.000000
	C	-1.242413	-0.736501	0.000000
	C	-2.408625	-1.468456	0.000000
	H	1.208936	-4.630066	0.000000
	H	-3.343177	-3.399274	0.000000
	H	-1.208936	-4.630066	0.000000
	C	1.225372	-3.551924	0.000000
	C	1.242413	-0.736501	0.000000
	H	-3.361484	-0.970270	0.000000
	C	2.408625	-1.468456	0.000000
	C	2.404604	-2.869323	0.000000
	H	3.361484	-0.970270	0.000000
	H	3.343177	-3.399274	0.000000
azulene				

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	C	0.000000	0.000000	-2.505949
	C	0.000000	-1.263159	-1.914657
	C	0.000000	-1.584690	-0.535873
	C	0.000000	1.263159	-1.914657
	C	0.000000	-0.733741	0.520585
	C	0.000000	1.584690	-0.535873
	C	0.000000	0.733741	0.520585
	H	0.000000	0.000000	-3.615872
	H	0.000000	-2.141954	-2.590022
	H	0.000000	-2.670249	-0.306783
	H	0.000000	2.141954	-2.590022
	H	0.000000	2.670249	-0.306783
	C	0.000000	-1.136561	1.921358
	H	0.000000	-2.173004	2.251274
	C	0.000000	0.000000	2.708171
	H	0.000000	0.000000	3.796664
	C	0.000000	1.136561	1.921358
	H	0.000000	2.173004	2.251274
C_2H_4				
	C	0.000000	0.000000	0.659674
	C	0.000000	0.000000	-0.659674
	H	0.000000	0.917277	1.224194
	H	0.000000	-0.917277	1.224194
	H	0.000000	0.917277	-1.224194
	H	0.000000	-0.917277	-1.224194
C_2H_3F				
	C	-0.006039	0.428293	0.000000
	C	1.165811	-0.153067	0.000000
	F	-1.148212	-0.267170	0.000000
	H	-0.179762	1.489041	0.000000
	H	1.257956	-1.224314	0.000000
	H	2.056146	0.447217	0.000000
1,1-$C_2H_2F_2$				
	C	0.000000	0.000000	1.366759
	C	0.000000	0.000000	0.069479
	H	0.000000	0.929658	1.900280
	H	0.000000	-0.929658	1.900280
	F	0.000000	1.073286	-0.689888
	F	0.000000	-1.073286	-0.689888
E-1,2-$C_2H_2F_2$				
	C	-0.391817	0.525462	0.000000
	C	0.391817	-0.525462	0.000000
	F	0.123791	1.752876	0.000000
	F	-0.123791	-1.752876	0.000000

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	H	-1.464760	0.489910	0.000000
	H	1.464760	-0.489910	0.000000
Z-1,2-$C_2H_2F_2$				
	C	0.000000	0.655882	0.571132
	C	0.000000	-0.655882	0.571132
	F	0.000000	1.373157	-0.544661
	F	0.000000	-1.373157	-0.544661
	H	0.000000	1.233825	1.475152
	H	0.000000	-1.233825	1.475152
C_2HF_3				
	C	-0.006784	0.420808	0.000000
	C	-0.701463	-0.685331	0.000000
	F	1.297883	0.492196	0.000000
	F	-0.561098	1.609870	0.000000
	F	-0.105646	-1.868134	0.000000
	H	-1.772692	-0.698209	0.000000
C_2F_4				
	C	0.000000	0.000000	0.653496
	C	0.000000	0.000000	-0.653496
	F	0.000000	1.089149	1.372397
	F	0.000000	-1.089149	1.372397
	F	0.000000	-1.089149	-1.372397
	F	0.000000	1.089149	-1.372397
pyridine				
	N	0.000000	0.000000	1.406386
	C	0.000000	0.000000	-1.370656
	C	0.000000	1.130835	0.717752
	C	0.000000	-1.130835	0.717752
	C	0.000000	1.185580	-0.668930
	C	0.000000	-1.185580	-0.668930
	H	0.000000	0.000000	-2.447849
	H	0.000000	2.043901	1.292092
	H	0.000000	-2.043901	1.292092
	H	0.000000	2.136767	-1.171486
	H	0.000000	-2.136767	-1.171486
butadiene				
	C	-0.398970	0.608901	0.000000
	C	0.398970	-0.608901	0.000000
	C	0.110840	1.831552	0.000000
	C	-0.110840	-1.831552	0.000000
	H	-1.470979	0.480141	0.000000
	H	1.470979	-0.480141	0.000000
	H	-0.519536	2.703162	0.000000
	H	1.175866	1.998710	0.000000

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	H	0.519536	-2.703162	0.000000
	H	-1.175866	-1.998710	0.000000
1,3-CHD				
	C	-0.062973	-1.412234	0.112250
	C	-0.109351	-0.723886	1.246213
	C	0.109351	0.723886	1.246213
	C	0.062973	1.412234	0.112250
	C	-0.250597	0.720934	-1.183391
	C	0.250597	-0.720934	-1.183391
	H	-0.193550	-2.481759	0.112811
	H	-0.291282	-1.218668	2.185505
	H	0.291282	1.218668	2.185505
	H	0.193550	2.481759	0.112811
	H	-1.334657	0.731277	-1.325298
	H	0.170929	1.264403	-2.023448
	H	-0.170929	-1.264403	-2.023448
	H	1.334657	-0.731277	-1.325298
furan				
	O	0.000000	0.000000	1.145633
	C	0.000000	1.083504	0.344768
	C	0.000000	-1.083504	0.344768
	C	0.000000	0.716000	-0.948558
	C	0.000000	-0.716000	-0.948558
	H	0.000000	2.032382	0.837737
	H	0.000000	-2.032382	0.837737
	H	0.000000	1.368499	-1.797526
	H	0.000000	-1.368499	-1.797526
thiophene				
	S	0.000000	0.000000	1.188266
	C	0.000000	1.231239	-0.012168
	C	0.000000	-1.231239	-0.012168
	C	0.000000	0.712855	-1.259714
	C	0.000000	-0.712855	-1.259714
	H	0.000000	2.263168	0.276152
	H	0.000000	-2.263168	0.276152
	H	0.000000	1.312484	-2.150984
	H	0.000000	-1.312484	-2.150984
o-benzyne				
	C	0.000000	0.698360	-1.055387
	C	0.000000	-0.698360	-1.055387
	C	0.000000	-1.437456	0.126485
	C	0.000000	-0.629137	1.240399
	C	0.000000	0.629137	1.240399
	C	0.000000	1.437456	0.126485

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	H	0.000000	1.218701	-1.998760
	H	0.000000	-1.218701	-1.998760
	H	0.000000	-2.512226	0.129780
	H	0.000000	2.512226	0.129780
m-benzyne				
	C	0.000000	1.183225	-0.640532
	C	0.000000	0.000000	-1.368871
	C	0.000000	-1.183225	-0.640532
	C	0.000000	-1.089698	0.722157
	C	0.000000	0.000000	1.551632
	C	0.000000	1.089698	0.722157
	H	0.000000	2.143409	-1.126034
	H	0.000000	0.000000	-2.447286
	H	0.000000	-2.143409	-1.126034
	H	0.000000	0.000000	2.623290
p-benzyne				
	C	0.000000	-1.335549	0.000000
	C	1.206179	-0.705475	0.000000
	C	1.206179	0.705475	0.000000
	C	0.000000	1.335549	0.000000
	C	-1.206179	0.705475	0.000000
	C	-1.206179	-0.705475	0.000000
	H	2.143716	-1.233116	0.000000
	H	2.143716	1.233116	0.000000
	H	-2.143716	1.233116	0.000000
	H	-2.143716	-1.233116	0.000000
1,8-NQ				
	C	0.000000	2.433241	-1.204923
	C	0.000000	1.212193	-1.842835
	C	0.000000	0.000000	-1.098520
	C	0.000000	0.000000	0.290566
	C	0.000000	1.272196	1.001592
	C	0.000000	2.469067	0.166741
	H	0.000000	-1.161054	-2.917752
	H	0.000000	3.344861	-1.775637
	H	0.000000	1.161054	-2.917752
	C	0.000000	-1.212193	-1.842835
	C	0.000000	-1.272196	1.001592
	H	0.000000	3.402432	0.703047
	C	0.000000	-2.469067	0.166741
	C	0.000000	-2.433241	-1.204923
	H	0.000000	-3.402432	0.703047
	H	0.000000	-3.344861	-1.775637
	O	0.000000	-1.409477	2.211344

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Table S2 – *Continued from previous page*

Molecule	Atom	X	Y	Z
	O	0.000000	1.409477	2.211344